

Energy levels of a two-dimensional hydrogen atom with spin-orbit Rashba interaction

C. Grimaldi

*Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str.38, D-01187 Dresden Germany
LPM, Ecole Polytechnique Fédérale de Lausanne, Station 17, CH-1015 Lausanne, Switzerland*

Electronic bound states around charged impurities in two-dimensional systems with structural inversion asymmetry can be described in terms of a two-dimensional hydrogen atom in the presence of a Rashba spin-orbit interaction. Here, the energy levels of the bound electron are evaluated numerically as a function of the spin-orbit interaction, and analytic expressions for the weak and strong spin-orbit coupling limits are compared with the numerical results. It is found that, besides the level splitting due to the lack of inversion symmetry, the energy levels are lowered for sufficiently strong spin-orbit coupling, indicating that the electron gets more tightly bound to the ion as the spin-orbit interaction increases. Similarities and differences with respect to the two-dimensional Fröhlich polaron with Rashba coupling are discussed.

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The two-dimensional (2D) hydrogen atom, *i. e.*, an electron constrained to move in a plane and subjected to an attractive Coulomb potential,^{1,2,3,4,5} is a theoretical construction which, besides being of interest in itself, has also important physical realizations. It can describe indeed the effect of a charged impurity in 2D systems such as quantum wells and surface states, or in extremely anisotropic three-dimensional crystals,¹ as well as excitons in semiconductor 2D heterostructures.⁵

The spin-orbit (SO) interaction, arising from the structural and/or bulk inversion asymmetries, characterizes several of the above mentioned low-dimensional systems,⁶ and gives rise to energy level splittings ranging from a few to hundreds of meV, depending on the material characteristics (see for example Ref.[7]). Furthermore, the possibility of tuning the SO interaction in semiconductor quantum wells by means of external applied voltages represents the key feature for application in spintronics. Given this situation, it becomes therefore natural to assess how the properties of a 2D hydrogen atom are affected by the SO interaction.

Several studies have already been devoted to the effect of the SO coupling in electrons interacting with central potentials, such as those describing hard-wall or parabolic quantum dots.^{8,9,10,11,12} However, despite its potential interest for SO coupled low-dimensional systems, the specific 2D Coulomb problem appears to have been only marginally considered in the literature.¹² In this Brief Report, the 2D Coulomb problem is numerically solved for an electron interacting with a Rashba potential, that is the SO coupling arising from structural inversion asymmetry in the direction perpendicular to the 2D plane.¹³ It is found that the Rashba interaction removes partially the initial degeneracy of the 2D hydrogen atom, and the resulting energy levels are two-fold degenerate due to the time-reversal invariance of the model. Furthermore, it is shown that the SO interaction renders the electron more tightly bound to the ion, confirming a general trend observed for other central potentials and for 2D electrons coupled to phonons.

The Hamiltonian for a 2D hydrogen atom in the pres-

ence of a Rashba SO potential is as follows ($\hbar = 1$):

$$H = \frac{\hat{p}^2}{2m_e} - \frac{Ze^2}{r} + \gamma(\hat{p}_x\sigma_y - \hat{p}_y\sigma_x), \quad (1)$$

where $\hat{p}_q = -i\partial/\partial q$ is the electron momentum operator ($q = x, y$), $\hat{p}^2 = \hat{p}_x^2 + \hat{p}_y^2$, m_e is the electron mass, and σ_x and σ_y are Pauli matrices. The last term of Eq.(1) describes the Rashba SO interaction with coupling parameter γ . For $\gamma \neq 0$ but zero Coulomb interaction ($Z = 0$), Eq.(1) is easily diagonalized in the momentum space, and the resulting energy dispersion of the free electron is composed of two branches $E_{k,\pm} = (k \pm k_R)^2/2m_e - E_R$, where $k_R = m_e\gamma$ is the Rashba momentum. In the ground state, the electron has energy $E_{k_R,-} = -E_R$, where $E_R = k_R^2/2m_e = m_e\gamma^2/2$.

In the presence of the Coulomb interaction, it is convenient to rewrite Eq.(1) in polar coordinates:

$$H = \begin{bmatrix} H_0 - \frac{Ze^2}{r} & -\gamma e^{-i\phi} \left(\frac{\partial}{\partial r} - \frac{i}{r} \frac{\partial}{\partial \phi} \right) \\ \gamma e^{i\phi} \left(\frac{\partial}{\partial r} + \frac{i}{r} \frac{\partial}{\partial \phi} \right) & H_0 - \frac{Ze^2}{r} \end{bmatrix}, \quad (2)$$

where

$$H_0 = -\frac{1}{2m_e} \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2} \right) \quad (3)$$

is the free electron Hamiltonian. Equation (2) commutes with the z -projection of the total angular momentum $\hat{J}_z = \hat{L}_z + \sigma_z/2$, where $\hat{L}_z = -i\partial/\partial\phi$, so that the eigenfunctions of (2) can be chosen to be simultaneously eigenfunctions of \hat{J}_z . Since H in polar coordinates allows for separation of variables, its eigenfunctions have therefore the following form:^{8,9,10,11,12}

$$\Psi_j(r, \phi) = \begin{bmatrix} f_j^-(r)e^{i(j-1/2)\phi} \\ f_j^+(r)e^{i(j+1/2)\phi} \end{bmatrix} \quad (4)$$

where $j = \pm 1/2, \pm 3/2, \dots$ are the eigenvalues of \hat{J}_z . The lack of spatial inversion symmetry induced by the presence of the Rashba interaction lowers the symmetry of

H when $\gamma \neq 0$. As shown below, this will induce a splitting of the energy levels compared to the case when $\gamma = 0$. Note however that H commutes with the time-reversal operator $\hat{K} = i\sigma_y \hat{C}$, where \hat{C} is the operation of complex conjugation, so that Ψ_j and its Kramer conjugate $\hat{K}\Psi_j$ have the same energy. This implies that, since $\hat{J}_z\Psi_j = j\Psi_j$ and $\hat{J}_z\hat{K}\Psi_j = -j\hat{K}\Psi_j$, the energy spectrum of H is invariant under the change $j \rightarrow -j$.

For bound states, the Schrödinger equation $H\Psi_j = E\Psi_j$ is rewritten by introducing $q_0^2 = -2m_e E$ and the dimensionless radial variable $\rho = 2q_0 r$. By using Eq.(4) one therefore finds

$$\left[\frac{d^2}{d\rho^2} + \frac{1}{\rho} \frac{d}{d\rho} - \frac{(j - 1/2)^2}{\rho^2} + \frac{\lambda}{2q_0\rho} - \frac{1}{4} \right] f_j^- + \frac{k_R}{q_0} \left(\frac{d}{d\rho} + \frac{j + 1/2}{\rho} \right) f_j^+ = 0, \quad (5)$$

$$\left[\frac{d^2}{d\rho^2} + \frac{1}{\rho} \frac{d}{d\rho} - \frac{(j + 1/2)^2}{\rho^2} + \frac{\lambda}{2q_0\rho} - \frac{1}{4} \right] f_j^+ - \frac{k_R}{q_0} \left(\frac{d}{d\rho} - \frac{j - 1/2}{\rho} \right) f_j^- = 0, \quad (6)$$

where $\lambda = 2m_e Ze^2$. The first terms in Eqs.(5) and (6) represent the differential equations for the radial wave function of the usual 2D Coulomb problem (*i.e.*, without SO coupling) with quantum numbers $j - 1/2$ and $j + 1/2$, respectively.^{2,3} Apart from a normalization constant, their solutions are of the form $R_{N,j\pm 1/2}(\rho) = \exp(-\rho/2)\rho^{|j\pm 1/2|}L_N^{2|j\pm 1/2|}(\rho)$ where $N = 0, 1, 2, \dots$ is the radial quantum number and $L_N^{2|j\pm 1/2|}(\rho)$ are Laguerre polynomials.^{2,5} The corresponding energy levels are

$$E_{N,j\pm 1/2}^0 = -\frac{\eta/4}{(N + |j \pm \frac{1}{2}| + \frac{1}{2})^2}, \quad (7)$$

where $\eta = 2m_e Z^2 e^4 = \lambda^2/2m_e$. By introducing the principal quantum number $n = N + |j \pm 1/2| = 0, 1, 2, \dots$, with $|j \pm 1/2| \leq n$, one infers that each level with fixed n has energy $-\eta/(2n + 1)^2$ with degeneracy $2(2n + 1)$.

For nonzero SO coupling, it is natural to expand the radial functions f_j^\pm in terms of $R_{N,j\pm 1/2}(\rho)$. By keeping in mind that the total wave function Ψ_j must be also eigenfunction of \hat{J}_z , one has:

$$f_j^\pm(\rho) = e^{-\rho/2}\rho^{|j\pm 1/2|} \sum_{N=0}^{\infty} A_{N,j}^\pm L_N^{2|j\pm 1/2|}(\rho). \quad (8)$$

By substituting the above expansions in Eqs.(5) and (6), and by making use of the properties of the Laguerre polynomials,¹⁴ one arrives at the following iterative system of equations

$$\left(\frac{\lambda}{2q_0} - \frac{1}{2} - |j - \frac{1}{2}| - N \right) A_{N,j}^- + \frac{k_R}{2q_0} C_{N',N}^j A_{N',j}^+ = 0, \quad (9)$$

$$\left(\frac{\lambda}{2q_0} - \frac{1}{2} - |j + \frac{1}{2}| - N \right) A_{N,j}^+ - \frac{k_R}{2q_0} C_{N',N}^{-j} A_{N',j}^- = 0, \quad (10)$$

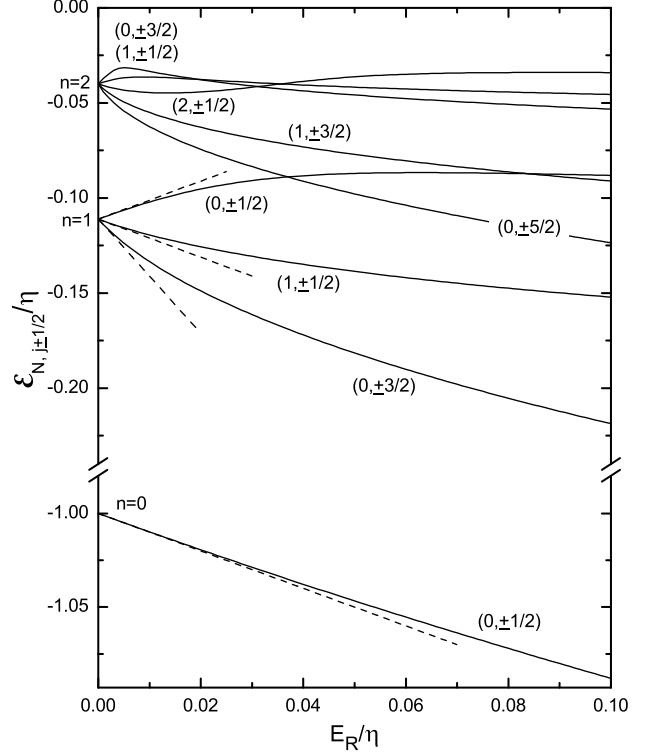


FIG. 1: Energy levels obtained from a numerical solution of Eqs.(9) and (10) (solid lines) as a function of the Rashba energy E_R . The dashed lines are the analytic results of Eq.(13) for the weak SO limit. All energy levels are shifted with respect to the ground state of the free electron with SO interaction [Eq.(14)]. The different levels are labeled by the principal quantum number n , reported in the left axis, and by the radial quantum number N and the total angular momentum in the z direction j reported in parentheses.

where

$$\begin{aligned} C_{N',N}^j = & \theta(j)[(N + 2j + 1)(N + 2j)\delta_{N',N} \\ & - N(N - 1)\delta_{N',N-2}] \\ & + \theta(-j)[\delta_{N',N+2} - \delta_{N',N}]. \end{aligned} \quad (11)$$

The values of q_0 , and so the energy levels $E = -q_0^2/2m_e$, satisfying Eqs.(9) and (10) can be easily obtained analytically in the limit of weak SO coupling. It suffices to recognize that decoupling Eqs.(9) and (10) leads to two iterative equations of the form $a_\pm A_{N,j}^\pm + b_\pm A_{N-2,j}^\pm + c_\pm A_{N+2,j}^\pm = 0$, whose solutions in the weak SO limit are determined simply by the condition $a_\pm = 0$, since b_\pm and c_\pm are both of order $(k_R/\lambda)^2$. Up to order $(k_R/\lambda)^2$ the coefficients a_\pm are given by

$$\begin{aligned} a_\pm = & \frac{\lambda}{2q_0} - \left(N + |j \pm \frac{1}{2}| + \frac{1}{2} \right) \\ & \mp \left(\frac{2k_R}{\lambda} \right)^2 \left(N + |j \pm \frac{1}{2}| + \frac{1}{2} \right)^3 \left(j \mp \frac{1}{2} \right), \end{aligned} \quad (12)$$

so that the energy levels $E_{N,j\pm 1/2}$ of the weak SO interacting case are

$$E_{N,j\pm 1/2} = E_{N,j\pm 1/2}^0 \pm 2jE_R - E_R, \quad (13)$$

where $E_{N,j\pm 1/2}^0$ is the energy spectrum for zero SO interaction given in Eq.(7). From Eq.(13) one sees therefore that the $2(2n+1)$ -fold degeneracy for zero SO coupling is lifted when $\gamma \neq 0$ and that each level is splitted into $2n+1$ levels, each two-fold degenerate. The remaining degeneracy is due to the time-reversal invariance of H and can be removed by adding a time-reversal breaking term in the Hamiltonian such as a magnetic field. Note also that Eq.(13) could be obtained by making use of the method described in Ref.[15].

A comparison between the weak SO coupling result (13) (dashed lines) and the energy levels obtained by a numerical solution of Eqs.(9) and (10) (solid lines) is reported in Fig.1 for a few energy levels. The principal quantum number values n are reported in the left axis, while the radial and total angular momentum quantum numbers N and j are indicated in parentheses. What is plotted in Fig.1 is actually the quantity

$$\mathcal{E}_{N,j\pm 1/2} = E_{N,j\pm 1/2} + E_R, \quad (14)$$

that is the energy spectrum shifted with respect to the ground state $-E_R$ of the free electron coupled to the SO potential. As it is shown in the figure, the ground state (identified by quantum numbers $n = 0$, $N = 0$, and $j = \pm 1/2$) has its energy lowered by the SO interaction, demonstrating that the electron gets more tightly bounded as E_R increase. This holds true also for the higher energy levels which, besides being splitted by the Rashba interaction, have their energies lowered for sufficiently large E_R values, as it apparent for most of the levels plotted in Fig.1. For states like $n = 1$ ($0, \pm 1/2$) and $n = 2$ ($2, \pm 1/2$) one needs $E_R/\eta \gtrsim 2$ before reaching net energy levels lower than the zero SO limit. This is of course unattainable since, for an unscreened charged impurity, η is of the order of one Ry, while the maximum value of E_R to date is of about 0.2 eV.¹⁶ The relevant values of E_R/η are therefore lower than about 0.01 for which, however, the perturbative result (14) is in quantitative good agreement with the numerical solution plotted in Fig.1.

Let us now discuss the relevance of the above results with respect to a different but somewhat related problem: that of a 2D electron strongly coupled to longitudinal optical phonons in the presence of a SO Rashba potential (Fröhlich-Rashba model).¹⁷ To this end it is useful to compare the exact numerical solutions of Eqs.(9) and (10) with a variational calculation of the ground state energy \mathcal{E}_0 obtained from the following electron trial wave function:

$$\Psi_0(r, \phi) = \mathcal{A}e^{-ar} \begin{bmatrix} J_0(br) \\ J_1(br)e^{i\phi} \end{bmatrix}, \quad (15)$$

where a and b are variational parameters, J_0 and J_1 are Bessel functions, and \mathcal{A} is a normalization constant. The

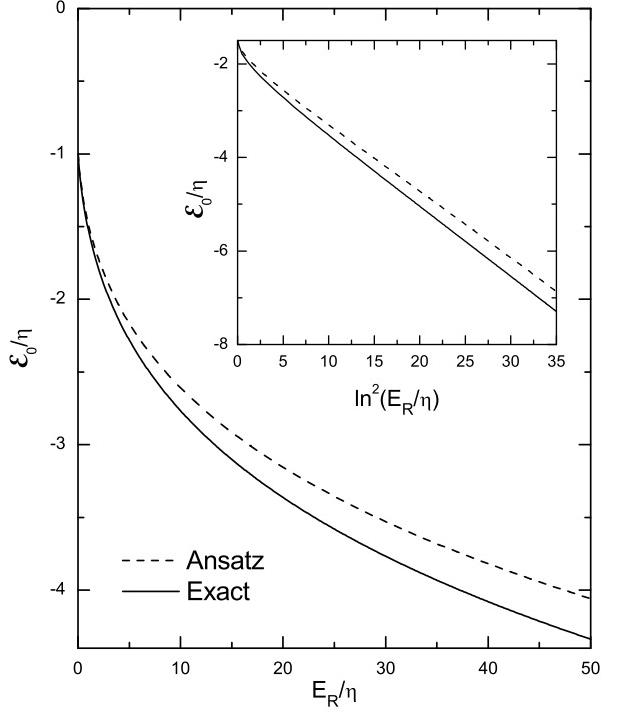


FIG. 2: Comparison between the exact ground state energy obtained from a numerical solution of Eqs.(9) and (10) (solid line) and the variational calculation with the ansatz wave function (15) (dashed line). Inset, the same results plotted as a function of $\ln^2(E_R/\eta)$.

above form for $\Psi_0(r, \phi)$ was introduced in Ref.[17] in order to find an upper bound for the ground state of a the Fröhlich-Rashba model. By using Eq.(15), the energy functional $\mathcal{F} = \langle \Psi_0 | (H + E_R) | \Psi_0 \rangle$ can be found analytically

$$\mathcal{F} = \frac{a^2}{2m_e} + \frac{(b - k_R)^2}{2m_e} + \frac{\lambda a}{m_e} \left[1 + \frac{K(ib/a)(b/a)^2}{K(ib/a) - E(ib/a)} \right], \quad (16)$$

where K and E are complete elliptic integrals of the first and second kind, respectively. Numerical minimization of Eq.(16) with respect to a and b provides an upper bound \mathcal{E}_0 for the ground state energy. This is plotted in Fig.2 by the dashed line and compared with the exact ground state energy (solid line) obtained from Eqs.(9) and (10). It is seen that the simple ansatz (15) reproduces fairly well the lowering of the ground state energy as E_R increases. In particular, by expanding Eq.(16) for small values of E_R compared to $\eta = \lambda^2/2m_e$ it turns out that $\mathcal{E}_0 \simeq -\eta - E_R$, which coincides with Eqs.(13) and (14) for $n = 0$, $N = 0$ and $j = 1/2$. For very large values of E_R/η , Eq.(16) has the limiting form

$$\mathcal{F} = \frac{a^2}{2m_e} + \frac{(b - k_R)^2}{2m_e} + \frac{\lambda a}{m_e} \ln\left(\frac{ea}{4b}\right), \quad (17)$$

where e is the Neper number and should not be confused with the electron charge. Equation (17) is min-

imized by setting $b = k_R$ and, within logarithmic accuracy, $a \simeq \lambda \ln(4k_R/\lambda e^2)$. Hence, the corresponding asymptotic upper bound for the ground state energy reduces to:

$$\mathcal{E}_0 \simeq -\eta \ln^2 \left(\frac{4k_R}{\lambda e^2} \right) = -\frac{\eta}{4} \ln^2 \left(\frac{16E_R}{\eta e^4} \right), \quad (18)$$

indicating that for $E_R \rightarrow \infty$ the ground state energy gets indefinitely lowered by following a squared logarithmic dependence on E_R . This result is confirmed in the inset of Fig.2, where both the exact result (solid line) and the numerical minimization of (16) (dashed line) reduce to straight lines when plotted as a function of $\ln^2(E_R/\eta)$.

The functional dependence of the ground state energy on the SO coupling shown in Eq.(18) was originally obtained by a different method in Ref.[12] where, however, a cutoff parameter was introduced to prevent a diverging result. As further noted in Ref.[12], a squared logarithmic behavior characterizes also the ground state energy of the

three-dimensional (3D) hydrogen atom in an extremely strong magnetic field H ,^{18,19} supporting the interpretation that a 2D electron in the presence of a strong Rashba SO interaction behaves effectively as a one-dimensional (1D) particle. The correspondence between 1D-like behavior and strong Rashba interaction has been noticed also for bound states of 2D electrons in short range central potentials,^{12,20} as well as for 2D electrons coupled to phonons.^{7,17} Such correspondence however does not appear to have universal validity. In fact when the ansatz (15) is used in the 2D Fröhlich-Rashba model, the asymptotic strongly-coupled polaron ground state energy for $E_R \rightarrow \infty$ does not decrease indefinitely as Eq.(18) but, rather, it reaches a minimum finite value.¹⁷ This is in striking contrast with the 3D strongly coupled Fröhlich polaron in a strong magnetic field, whose ground state energy has a squared logarithmic functional form as the 3D hydrogen atom for $H \rightarrow \infty$,²¹ due to the 1D confining effect of the magnetic field on the electron motion.

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